

## Effects of additional volatile organic compounds, organic nitrates and oxygenated organic species on global tropospheric chemistry

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It is widely recognized that volatile organic compounds have a large influence on the photochemistry of the remote troposphere. The volatile organics are known to directly affect the chemistry of O<sub>3</sub>, nitrates and OH, and are also linked to the chemistry of CO and CH<sub>4</sub>. This work evaluates the sensitivity of tropospheric ozone and its precursors to the representation of non-methane volatile organic compounds (NMVOCs) and organic nitrates. A global 3-D tropospheric chemistry/transport model (IMPACT), which was developed at the Lawrence Livermore National Laboratory (LLNL) [Rotman et al., 2004] and subsequently modified at the University of Michigan [e.g. Wallington et al., 2005], has been exercised previously under the NASA Global Modeling Initiative (GMI) [Rodriguez et al., 2004] using the GEOS-CHEM chemical reaction mechanism, which has been widely used in global modeling studies [e.g. Bey et al., 2001]. In this work, the model was extended by adding emissions and photochemical reactions for aromatic and terpenoid hydrocarbons, and by adding explicit representation of hydroxy alkyl nitrates produced from isoprene. Emissions of methanol, phenol, acetic acid and formic acid associated with biomass burning were also added. Results show that O<sub>3</sub> increases by 20% in most of the troposphere, peroxyacetyl nitrate (PAN) increases by 30% over much of the troposphere and OH increases by 10%. NO<sub>x</sub> (NO + NO<sub>2</sub>) decreases near source regions and increases in remote locations, reflecting increased transport of NO<sub>x</sub> away from source regions by organic nitrates. The increase in O<sub>3</sub> was driven largely by the increased role of PAN as a transporter of NO<sub>x</sub> and by the re-release of NO<sub>x</sub> from isoprene nitrates. The increased PAN (CH<sub>3</sub>C(O)OONO<sub>2</sub>) production was associated with increases in methyl glyoxal (CH<sub>3</sub>COCHO) and hydroxyacetone (HOCH<sub>2</sub>C(O)CH<sub>3</sub>). Comparison with measured values show reasonable agreement for O<sub>3</sub> and PAN, but model-measurement agreement does not either improve or degrade in the extended model. The extended model shows improved agreement with measurements for methanol, acetic acid and peroxypropional nitrate (PPN). Results from the extended model were consistent with measured alkyl nitrates, but hydroxyacetone was overestimated and hydroxyacetaldehyde (HOCH<sub>2</sub>CHO) was underestimated, suggesting that the latter may be a reaction product of the hydroxyalkyl nitrates.

### References

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